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The Inversion, Analysis, and Assimilation problems

Part 1

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1. Introduction

The literatures of the satellite radiance problem and the sonde height analysis problem have such different terminologies that the connection between the two problems is obscured. The purpose of this note is to point up the connection between the two types of problem as it is thought that this may well assist the development of a viable 4-d assimilation scheme.

Throughout the main part of the text one set of notation has been used for both problems. Although it is the meteorological inversion and analysis problems which are in mind in this text, reference being specifically made to them in places, the note is written from a wider standpoint. Thus when the word "ANALYSIS" occurs in the text it means a problem in which there are more equations of condition than unknowns. The word "INVERSION" in the text implies a problem in which there are fewer equations of condition than unknowns. This is thus a fairly general exposition which is entirely without prejudice to anybody else's view as to how inversion, analysis, and assimilation should be tackled.

One or two specific proposals on the assimilation problem in the light of this note will be put forward in Part 2.

N.B. This paper has not been published. Permission to quote from it must be obtained from the Assistant Director of the above Meteorological Office branch.

2. The Analysis and Inversion Problems

The ANALYSIS problem is

$$\underset{ml}{h} = \underset{mn}{F}.\underset{nl}{a} + \underset{ml}{r} \qquad m > n \qquad (1)$$

where

$\underset{ml}{h}$ is the mxl column vector of heights or temps.

$\underset{mn}{F}$ is the mxn information density matrix of function evaluations over the domain.

$\underset{nl}{a}$ is the nxl column vector of unknown coeffs. which have to be determined.

$\underset{ml}{r}$ is the mxl column vector of residuals

The INVERSION problem is

$$\underset{ml}{i} = \underset{mn}{K}.\underset{nl}{b} + \underset{ml}{o} \qquad m < n \qquad (2)$$

where

$\underset{ml}{i}$ is the mxl column vector of radiances

$\underset{mn}{K}$ is the mxn weighting function matrix

$\underset{nl}{b}$ is the nxn column vector of unknown coeffs. which have to be determined

$\underset{ml}{o}$ is the (ideally) zero mxl column vector of residuals

In the ANALYSIS problem the essential difficulty is that in a problem of any size the matrix F is likely to be ill-conditioned and in the equations governing the propagation of round-off error the condition number of the matrix F acts as an amplifying factor resulting in a highly unreliable solution vector. In the ANALYSIS problem, provided that F is not actually singular, we may overcome this difficulty by an appropriately implemented Gram-Schmidt type of factorization of F.

In the INVERSION problem the essential difficulty is that as we have a situation in which there are more unknowns than equations ($m < n$) there exists not one solution but an infinity of solutions, most of which will be physically unrealistic. The difficulty is aggravated by the influence of noise in the data, and it is so severe that, for the most part, direct methods of solution corresponding to that indicated above for the analysis type of problem have not found much favour. In operational practice, so far, indirect methods involving regression relationships with sonde data have been preferred.

In what follows, to avoid complicating the notation we will deal simply with the one vector-matrix equation

$$\underset{ml}{h} = \underset{mn}{F}.\underset{nl}{a} + \underset{ml}{r} \qquad (3)$$

where if we are dealing with the ANALYSIS problem $\underline{h}$ is the observed heights or temps vector, F is the information density matrix, and $\underline{r}$ is the residual vector. If we are dealing with the INVERSION problem then $\underline{h}$ is the vector of radiances, F is the weighting function matrix and $\underline{r}$ is the residual vector which ideally would be zero. $\underline{a}$ is the solution vector in both cases. Which case is being dealt with will be made explicitly clear in the text. The essential point is that in the ANALYSIS problem we have $m > n$, whilst in the INVERSION problem we have $m < n$.

Before beginning the exposition of the unified mathematical approach to the solution of both these problems it is necessary to make the point that in the INVERSION case ($m < n$) despite the infinity of solutions there is nevertheless one unique solution and this one can be found. To illustrate what is meant by this statement suppose that we have four bits of data h_1, h_2, h_3, and h_4, and that we decide to fit to them the quartic polynomial

$$z = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 \qquad (4)$$

Putting the values h_1, h_2, h_3, h_4 into (4) in turn we get the four equations of condition

$$\begin{aligned} h_1 &= a_0 + a_1 x_1 + a_2 x_1^2 + a_3 x_1^3 + a_4 x_1^4 \\ h_2 &= a_0 + a_1 x_2 + a_2 x_2^2 + a_3 x_2^3 + a_4 x_2^4 \\ h_3 &= a_0 + a_1 x_3 + a_2 x_3^2 + a_3 x_3^3 + a_4 x_3^4 \\ h_4 &= a_0 + a_1 x_4 + a_2 x_4^2 + a_3 x_4^3 + a_4 x_4^4 \end{aligned} \qquad (5)$$

As we then have 4 equations and 5 unknown coeffs. the system is apparently insoluble because we have arrived at the position illustrated in Figure 1, with an infinite number of such polynomials satisfying the data

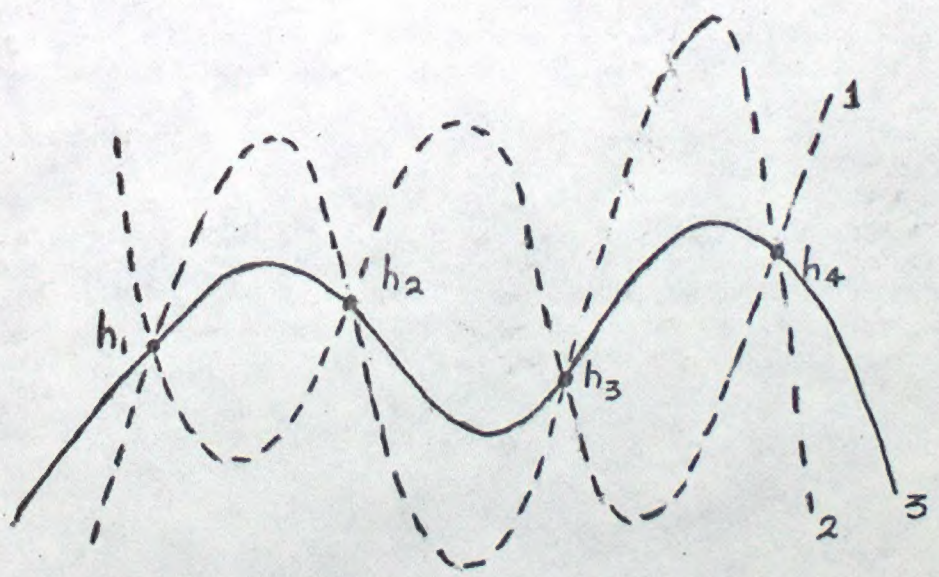

Figure 1

Writing the fitting polynomial (4) as

$$z = \tilde{\underline{f}} \cdot \underline{a}$$

where

$\tilde{\underline{f}}$ is the vector $(1, x, x^2, x^3, x^4)$

$\underline{a}$ is the vector $(a_0, a_1, a_2, a_3, a_4)^{\sim}$

and $\cdot$ indicates the scalar product

the difficulty is that there is an infinity of coeff. vectors $\underline{a}$ which yield polynomials going through the h values. However, a mathematically unique solution exists because out of the infinity of $\underline{a}$ - vectors we may select the one which has minimum Euclidean length. That is, we may find the solution vector $\underline{a}$ having the property that

$$|\underline{a}| = \sqrt{a_0^2 + a_1^2 + a_2^2 + a_3^2 + a_4^2}$$

is a minimum. It can be shown that there is just one such $\underline{a}$. We will take the solid line in Figure 1 as illustrating this particular solution.

The special property of this particular solution vector $\underline{a}$ is that it is the one which, inserted in (4), yields the smoothest of the infinity of possible fitting polynomials. Alternatively it may be expressed that in the absence of any information other than the h values this particular $\underline{a}$ yields the greatest justifiable degree of resolution in the solution.

Note that it is not claimed that this particular minimum $|\underline{a}|$ solution is the "best" solution to the problem in any physical sense. There are very likely better solutions amongst the infinity, but to find them some knowledge additional to the h values has to be brought in. This additional knowledge is then formulated in such a way as to provide one or more extra equations of condition to be added to (5), converting the system into a 5 x 5 or an m x 5, with $m > 5$. It is not even claimed that this minimum $|\underline{a}|$ solution is a usable solution. The circumstances of the physical problem may be such that the min $|\underline{a}|$ solution is simply not good enough and additional information must be used. However, in this case the normative role of the min $|\underline{a}|$ solution should not be overlooked. In view of its properties it may be desirable to know how far the solution actually used departs from it. If we denote the min $|\underline{a}|$ solution by $\underline{a}_{min}$, then if some other solution say, $\underline{a}_j$ is used, then $|\underline{a}_j - \underline{a}_{min}|$ is a valuable indicator of the degree of dependency of the solution on additional information. This aspect of $\underline{a}_{min}$ is very relevant to the assimilation problem because here it is highly probable that the additional information may be supplied by the model itself, in which case $|\underline{a}_j - \underline{a}_{min}|$ monitors the model dependency of the process, or to put it another way it must be remembered that $\underline{a}_{min}$ represents the genuinely model independent information going into the process.

We begin the presentation of the unified approach by deriving the traditional solutions to both types of problem on the assumption that F is of full rank. That is to say that in the ANALYSIS problem ($m > n$) we assume that rank F is n, and that in the INVERSION problem ($m < n$) we assume rank F is m.

The ANALYSIS problem ($m > n$) is specified by

$$\underset{ml}{\underline{h}} = \underset{mn}{F} \cdot \underset{nl}{\underline{a}} + \underset{ml}{\underline{r}} \qquad (6)$$

$$\underset{n1}{o} = \underset{nm}{\tilde{F}} \cdot \underset{m1}{r} \tag{7}$$

(7) is the condition which ensures the least-squares solution. Using it, we obtain from (6) the Normal Equations

$$(\underset{nm}{\tilde{F}} \cdot \underset{mn}{F}) \cdot \underset{n1}{a} = \underset{nm}{\tilde{F}} \cdot \underset{m1}{h} \tag{8}$$

yielding

$$\underset{n1}{a} = (\underset{nm}{\tilde{F}} \cdot \underset{mn}{F})^{-1} \cdot \underset{nm}{\tilde{F}} \cdot \underset{m1}{h} \tag{9}$$

In the INVERSION problem ($m < n$) we have

$$\underset{m1}{h} = \underset{mn}{F} \cdot \underset{n1}{a} + \underset{m1}{r} \tag{10}$$

and, assuming that we are content to have the data fitted exactly

$$\underset{m1}{r} = \underset{m1}{o} \tag{11}$$

We may then rewrite (10) as

$$\underset{mm}{I} \cdot \underset{m1}{h} = \underset{mn}{F} \cdot \underset{n1}{a} \tag{12}$$

since multiplying the L.H.S. by the Idemfactor (unit matrix) I changes nothing. Then since F is of full rank the Idemfactor in (12) may be expressed as

$$\underset{mm}{I} = (\underset{mn}{F} \cdot \underset{nm}{\tilde{F}}) \cdot (\underset{mn}{F} \cdot \underset{nm}{\tilde{F}})^{-1} \tag{13}$$

so that (12) becomes

$$(\underset{mn}{F} \cdot \underset{nm}{\hat{F}}) \cdot (\underset{mn}{F} \cdot \underset{nm}{\tilde{F}})^{-1} \cdot \underset{m1}{h} = \underset{mn}{F} \cdot \underset{n1}{a} \tag{14}$$

the terms of which may be regrouped to give

$$\underset{mn}{F} \cdot \underset{n1}{a} = \underset{mn}{F} \cdot \left[\underset{nm}{\tilde{F}} \cdot (\underset{mn}{F} \cdot \underset{nm}{\hat{F}})^{-1} \cdot \underset{m1}{h} \right] \tag{15}$$

which, because F is full rank, yields

$$\underset{n1}{a} = \underset{nm}{\hat{F}} \cdot (\underset{mn}{F} \cdot \underset{nm}{\tilde{F}})^{-1} \cdot \underset{m1}{h} \tag{16}$$

It is convenient for ease of reference and comparison to bring these two solutions (9) and (16) together

ANALYSIS $(m > n)$	$\underset{n1}{a} = (\underset{nm}{\hat{F}} \cdot \underset{mn}{F})^{-1} \cdot \underset{nm}{\tilde{F}} \cdot \underset{m1}{h}$	(9)
INVERSION $(m < n)$	$\underset{n1}{a} = \underset{nm}{\hat{F}} \cdot (\underset{mn}{F} \cdot \underset{nm}{\tilde{F}}) \cdot \underset{m1}{h}$	(16)

Some points may be noted

(i) In most real-life problems the straightforward use of these traditional formulae will be disastrous even though F is full rank.

(ii) In the ANALYSIS problem the inverse $(\tilde{F}.F)^{-1}$ is an <u>exterior</u> factor on the R.H.S. In the INVERSION problem the inverse $(F.\tilde{F})^{-1}$ is an <u>interior</u> factor on the R.H.S. This fact alone tends to make the algebra of the INVERSION problem somewhat more awkward than that for the ANALYSIS case.

(iii) Both derivations fail totally if F is not of full rank.

The unified approach to these two problems is obtained by making use of the Singular Value Decomposition (SVD). This involves the factorization of the F matrix as

$$F = U \cdot \Lambda \cdot \tilde{V} \tag{17}$$

where U and V are respectively the domain-space and function-space modal matrices and Λ is the diagonal matrix $(\lambda_1, \lambda_2, \lambda_3, - - - - - -)$ of positive square-roots of eigenvalues of $(\tilde{F}.F)$ or $(F.\tilde{F})$. We may visualize the λ_i as having been arranged in descending order of magnitude. The modal matrices consist of the corresponding orthogonal columns of eigenvectors.

In the solution of the ANALYSIS problem ($m > n$) via SVD we have

$$\underset{m1}{h} = \underset{mn}{F} \cdot \underset{n1}{a} + \underset{m1}{r} \tag{18}$$

$$\underset{n1}{o} = \underset{nm}{\tilde{F}} \cdot \underset{m1}{r} \tag{19}$$

$$\underset{mn}{F} = \underset{mn}{U} \cdot \underset{nn}{\Lambda} \cdot \underset{nn}{\tilde{V}} \tag{20}$$

Using (19) and (20) in (18) gives

$$\underset{mn}{U} \cdot \underset{nn}{\Lambda} \cdot \underset{nn}{\tilde{V}} \cdot \underset{n1}{a} = \underset{m1}{h}$$

i.e. $$\underset{nn}{\Lambda} \cdot \underset{nn}{\tilde{V}} \cdot \underset{n1}{a} = \underset{nm}{\tilde{U}} \cdot \underset{m1}{h} \qquad \left(\text{because } \underset{nm}{\tilde{U}} \cdot \underset{mn}{U} = \underset{nn}{I}\right)$$

i.e. $$\underset{nn}{\tilde{V}} \cdot \underset{n1}{a} = \underset{nn}{\Lambda^{-1}} \cdot \underset{nm}{\tilde{U}} \cdot \underset{m1}{h}$$

and finally because $$\underset{nn}{V} \cdot \underset{nn}{\tilde{V}} = \underset{nn}{I}$$

$$\underset{n1}{a} = \underset{nm}{V} \cdot \underset{nn}{\Lambda^{-1}} \cdot \underset{nm}{\tilde{U}} \cdot \underset{m1}{h} \tag{21}$$

In the solution of the INVERSION problem ($m < n$) via SVD we have

$$\underset{ml}{h} = \underset{mn}{F} \cdot \underset{nl}{a} + \underset{ml}{r} \tag{22}$$

$$\underset{ml}{r} = \underset{ml}{o} \tag{23}$$

$$\underset{mn}{F} = \underset{mm}{U} \cdot \underset{mn}{\Lambda} \cdot \underset{mn}{\widetilde{V}} \tag{24}$$

Using (23) and (24) in (22) we get

$$\underset{mm}{U} \cdot \underset{mn}{\Lambda} \cdot \underset{mn}{\widetilde{V}} \cdot \underset{nl}{a} = \underset{ml}{h}$$

i.e. $$\underset{mn}{\Lambda} \cdot \underset{mn}{\widehat{V}} \cdot \underset{nl}{a} = \underset{mm}{\widetilde{U}} \cdot \underset{ml}{h} \qquad (\text{because } \underset{mm}{\widetilde{U}} \cdot \underset{mm}{U} = \underset{mm}{I})$$

$$\underset{mn}{\widehat{V}} \cdot \underset{nl}{a} = \underset{mn}{\Lambda^{-1}} \cdot \underset{mm}{\widetilde{U}} \cdot \underset{ml}{h} \tag{25}$$

and now we come to a subtlety of the INVERSION case. In this case $\underset{nm}{V} \cdot \underset{mn}{V} = \underset{nn}{I}$ is *not* true and so we cannot use this to get from (25) to the solution for $\underset{nl}{a}$. On the other hand $\underset{nm}{V} \cdot \underset{mn}{\widetilde{V}}$ is a projection matrix which projects $\underset{nl}{a}$ on to a vector space in which $\underset{nl}{a}$ already lies. Hence

$$\left(\underset{nm}{V} \cdot \underset{mn}{\widetilde{V}}\right) \cdot \underset{nl}{a} = \underset{nl}{a} \tag{26}$$

and this fact serves instead. Using (26) and (25) we have

$$\underset{nl}{a} = \underset{nm}{V} \cdot \underset{mn}{\Lambda^{-1}} \cdot \underset{mm}{\widetilde{U}} \cdot \underset{ml}{h} \tag{27}$$

and we see that, formally, this INVERSION solution (27) is the same as the ANALYSIS solution (21).

It is not immediately obvious that the solutions (21) and (27) are the same as their traditional counterparts (9) and (16) but by using the SVD for F in (9) and (16) the equivalences are soon established. (27) gives the shortest length solution of all possible solutions to (22). A rigorous proof of this will not be given here, but it is a well-known result and a visualization of its truth is to be had as follows -

The general solution to (22), with $\underline{r} = o$, is given by

$$\overset{*}{\underline{a}} = \underline{a} + \overset{\vee}{\underline{a}} \tag{28}$$

where $\underline{a}$ is given by (27) and $\overset{\vee}{\underline{a}}$ is any vector orthogonal to the columns of F. It may be directly verified that (28) satisfies (22) subject to this condition. But this condition implies that $\overset{*}{a}^2 = a^2 + \overset{\vee}{a}^2$, and so the shortest solution is given by $\overset{*}{\underline{a}} = \underline{a}$. The only way that $\underline{a}$ itself could be shortened would be equivalent to setting one or more elements of Λ^{-1} equal to zero, but in this case $\underline{a}$ would no longer satisfy (22), with $\underline{r} = o$. (27) is therefore the minimum length solution.

In the ANALYSIS problem ($m > n$) specified by (6) and (7) we seek that solution which minimizes the sum of squares of residuals. Denote this by SSR_{min}. Using the SVD amounts to transforming the variables so that we have

$$\underset{nn}{\tilde{V}} \cdot \underset{n1}{a} = \underset{n1}{b} \tag{29}$$

and the inverse relationship

$$\underset{n1}{a} = \underset{nn}{V} \cdot \underset{n1}{b} \tag{30}$$

and the solution (21) becomes

$$\underset{n1}{b} = \underset{nn}{\Lambda^{-1}} \cdot \underset{nm}{\hat{U}} \cdot \underset{m1}{h} \tag{31}$$

Since Λ^{-1} is diagonal we can express (31) to give the individual elements of the coefficient vector $\underline{b}$ as

$$b_j = \frac{\hat{\underline{u}} \cdot \underline{h}}{\lambda_j} \qquad j = 1, 2, \cdots, n \tag{32}$$

and we can take the singular values λ_j as being in descending order of magnitude. The $\underline{u}_j$ are the corresponding transposed eigencolumns of the modal matrix U. The effect of the transformation has been to turn the system (18) into a decoupled one with the result that the b_j are independent of each other. This has the advantage that we can discard one without affecting the others. The successively smaller λ_j correspond to smaller and smaller scales in the data vector $\underline{h}$ and beyond a certain value $\lambda_j = \varepsilon$, determined by theoretical and physical arguments and/or experimental evidence, we can judge that the b_j in the tail of $\underline{b}$ are determined by noise rather than signal. If this is so, then it is seen from (30) that these noise determined tail-enders in the $\underline{b}$ vector contaminate the whole of the solution vector $\underline{a}$. A remedy then is to put

$$\begin{aligned} b_j &= \frac{\hat{\underline{u}}_j \cdot \underline{h}}{\lambda_j} && \text{if } \lambda_j \geqslant \text{some } \varepsilon \\ b_j &= 0 && \text{if } \lambda_j < \text{some } \varepsilon \end{aligned} \tag{33}$$

and by using the $\underline{b}$ vector thus determined we avoid contaminating $\underline{a}$ via (30). There is, however, a price to pay for this. It can be shown that SSR_{min} has the value

$$SSR_{min} = h^2 - b_1^2\lambda_1^2 - b_2\lambda_2^2 - \cdots\cdots - b_n^2\lambda_n^2 \tag{34}$$

so that if, on some judgment, we put $b_{j+1} = b_{j+2} = \cdots\cdots = b_n = 0$, then the sum of squares of residuals will be increased by

$$\Delta SSR = \sum_{i=j+1}^{i=n} b_i^2\lambda_i^2 = \sum_{i=j+1}^{i=n} (\underline{u}_i \cdot \underline{h})^2 \tag{35}$$

The solution $\underline{a}$ obtained by setting the noisy tail-enders in $\underline{b}$ to zero is not of course the same solution as obtained when not doing this. And it is not the solution corresponding to SSR_{min}. But if we have chosen ε correctly it is a relatively uncontaminated solution. We have a trade-off situation.

BENEFIT	COST
A more reliable solution vector $\underline{a}$, not so affected by noise in the data.	An increase in the SSR over and above the optimum least-squares value.

Turning again to the INVERSION ($m < n$) problem, eqns. (22), (23) and following, it is evident that we can take exactly the same view as in the analysis problem, namely, treat the SVD as a transformation of variables and then set the tail-enders in $\underline{b}$ to zero. There is a subtle difference. The minimum $|\underline{a}|$ solution (27) corresponds to $\underline{r} = \underline{o}$, i.e. we fit the data exactly and thus the "SSR" is zero and it is to this "SSR" = o datum that the cost/benefit trade-off position is related in this case. Thus when we zero the tail-end of $\underline{b}$, transform back to $\underline{a}$ (using $\underline{a} = V.\underline{b}$) we get not an $\underline{a}$ satisfying (22) with $\underline{r} = \underline{o}$, but an a^1 satisfying (22) with an $\underline{r} \neq \underline{o}$ such that

$$r^2 = b_{j+1}^2 \lambda_{j+1}^2 + b_{j+2}^2 \lambda_{j+2}^2 + \text{-------} + b_m^2 \lambda_m^2 \qquad (36)$$

or equivalently

$$r^2 = (\underline{U}_{j+1} \cdot \underline{b})^2 + (\underline{U}_{j+2} \cdot \underline{b})^2 + \text{---} + (\underline{U}_m \cdot \underline{b})^2 \qquad (37)$$

and the trade-off position is

BENEFIT	COST
A more reliable solution vector $\underline{a}$, not so affected by noise in the data	An increase in the "SSR" from zero to SSR = r^2 given by (36) or (37)

There is a traditional approach to the trade-off situation with respect to both types of problem, analysis and inversion, which is strongly related to the SVD method. This approach is known as Tychonov Regularization (and also as Ridge Analysis).

In the ANALYSIS problem ($m > n$) suppose that instead of solving

$$\underset{m1}{\underline{h}} = \underset{mn}{F} \cdot \underset{n1}{\underline{a}} + \underset{m1}{\underline{r}} \qquad (38)$$

we solve

$$\begin{pmatrix} \underline{h} \\ \hline \underline{o} \end{pmatrix} = \begin{pmatrix} F \\ \hline \mu I \end{pmatrix} \cdot \underline{a} + \underline{r}' \qquad (39)$$

The solution is given by the Normal equations

$$(\tilde{F} \,|\, \mu I) \cdot \begin{pmatrix} F \\ \hline \mu I \end{pmatrix} \cdot \underline{a} = (\tilde{F} \,|\, \mu I) \cdot \begin{pmatrix} \underline{h} \\ \hline \underline{o} \end{pmatrix} \qquad (40)$$

which comes to

$$(\underset{nm}{\tilde{F}} \cdot \underset{mn}{F} + \mu^2 \underset{nn}{I}) \cdot \underset{n1}{a} = \underset{nm}{\tilde{F}} \cdot \underset{m1}{h} \qquad (41)$$

and the solution is then

$$\underset{n1}{a} = (\underset{nm}{\tilde{F}} \cdot \underset{mn}{F} + \mu^2 \underset{nn}{I})^{-1} \cdot \underset{nm}{\tilde{F}} \cdot \underset{m1}{h} \qquad (42)$$

in which μ is a disposable scalar which has to be chosen so that the benefit of the easier and more reliable invertibility of $(\tilde{F}.F + \mu^2 I)$ as compared with $\tilde{F}.F$ is not offset by an unacceptable increase in the SSR over and above SSR_{min}.

If we put the SVD decomposition (20) into (41) there results

$$[(\underset{nn}{V} \cdot \underset{nn}{\Lambda} \cdot \underset{nm}{\tilde{U}}) \cdot (\underset{mn}{U} \cdot \underset{nn}{\Lambda} \cdot \underset{nn}{\tilde{V}}) + \mu^2 \underset{nn}{I}] \cdot \underset{n1}{a} = \underset{nn}{V} \cdot \underset{nn}{\Lambda} \cdot \underset{nm}{\tilde{U}} \cdot \underset{m1}{h} \qquad (43)$$

i.e.
$$(\underset{nn}{V} \cdot \underset{nn}{\Lambda^2} \cdot \underset{nn}{\tilde{V}} + \mu^2 \underset{nn}{I}) \cdot \underset{n1}{a} = \underset{nn}{V} \cdot \underset{nn}{\Lambda} \cdot \underset{nm}{\tilde{U}} \cdot \underset{m1}{h}$$

Taking $\underset{nn}{\tilde{V}}\cdot$ through this, there follows

$$(\underset{nn}{\Lambda^2} \cdot \underset{nn}{\tilde{V}} + \mu^2 \underset{nn}{\tilde{V}}) \cdot \underset{n1}{a} = \underset{nn}{\Lambda} \cdot \underset{nm}{\tilde{U}} \cdot \underset{m1}{h}$$

$$(\underset{nn}{\Lambda^2} + \mu^2 \underset{nn}{I}) \cdot \underset{nn}{\tilde{V}} \cdot \underset{n1}{a} = \underset{nn}{\Lambda} \cdot \underset{nm}{\tilde{U}} \cdot \underset{m1}{h}$$

and again putting $\underset{nn}{\tilde{V}} \cdot \underset{n1}{a} = \underset{n1}{b}$ we have

$$(\underset{nn}{\Lambda^2} + \mu^2 \underset{nn}{I}) \cdot \underset{n1}{b} = \underset{nn}{\Lambda} \cdot \underset{nm}{\tilde{U}} \cdot \underset{m1}{h}$$

so that, finally

$$\underset{n1}{b} = (\underset{nn}{\Lambda^2} + \mu^2 \underset{nn}{I})^{-1} \cdot (\underset{nn}{\Lambda} \cdot \underset{nm}{\tilde{U}} \cdot \underset{m1}{h}) \qquad (44)$$

which, componentwise, may be expressed as

$$b_j = \frac{\lambda_j}{\lambda_j^2 + \mu^2} (\underline{\tilde{u}}_j \cdot \underline{h}) \qquad j = 1, 2, \cdots, n \qquad (45)$$

The relationship between the SVD solution and the Tychonov Regularization solution is now clear, for we have

TYCHONOV

$$b_j = \frac{\lambda_j}{\lambda_j^2 + \mu^2} (\underline{\tilde{u}}_j \cdot \underline{h})$$

$$\Delta SSR = \sum_{i=1}^{i=n} \left[1 - \frac{\lambda_i^2}{\lambda_i^2 + \mu^2}\right] (\underline{\tilde{u}}_j \cdot \underline{h})^2$$

SVD

$$b_j = \frac{\underline{\tilde{u}}_j \cdot \underline{h}}{\lambda_j} \qquad \lambda_j \geq \varepsilon$$

$$b_j = 0 \qquad \lambda_j < \varepsilon$$

$$\Delta SSR = \sum_{i=j+1}^{i=n} (\underline{\tilde{u}}_j \cdot \underline{h})^2$$

and it is seen that the Tychonov solution is an approximation to the SVD solution. See Figure 2.

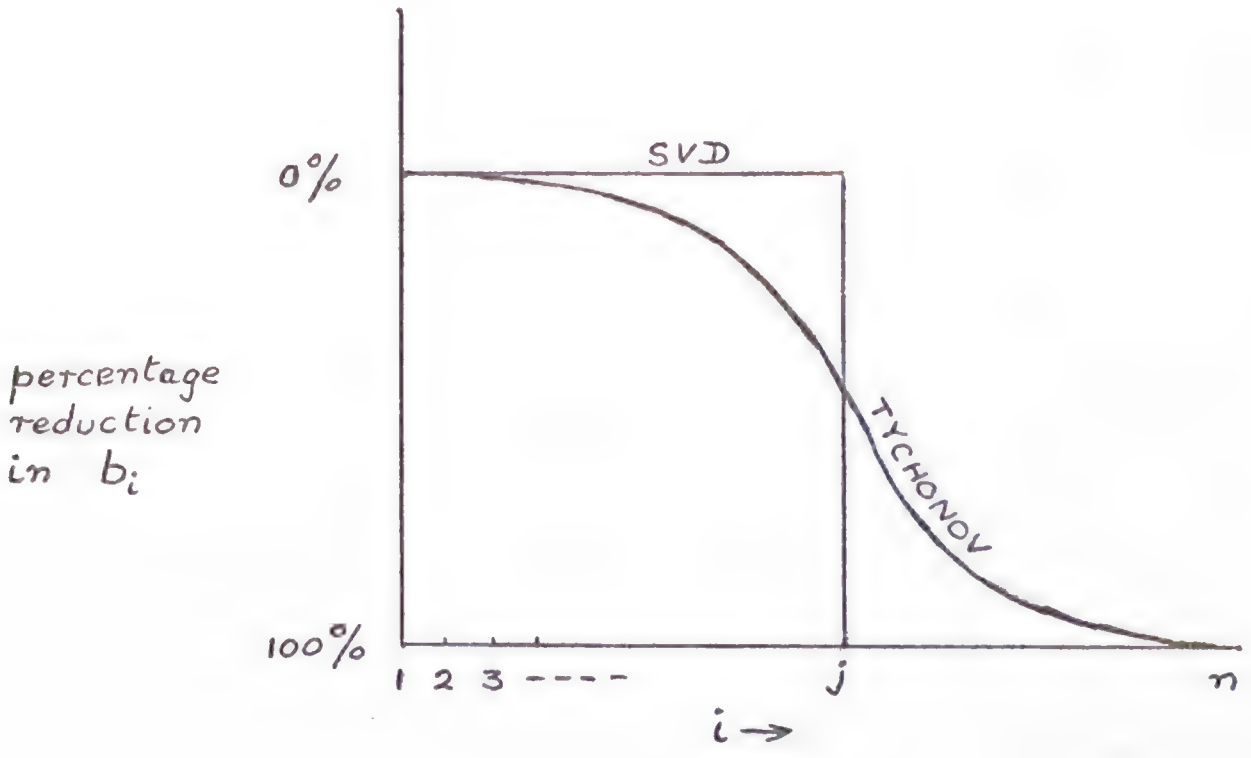

Figure 2

In the INVERSION problem (m < n) suppose that instead of solving

$$\underset{m1}{h} = \underset{mn}{F} \cdot \underset{n1}{a} + \underset{m1}{o} \tag{46}$$

we solve

$$\underset{m1}{h} = \left(\underset{mn}{F} \,\vdots\, \mu \underset{mm}{I}\right) \cdot \begin{pmatrix} \underset{n1}{a} \\ \cdots \\ \underset{m1}{o} \end{pmatrix} + \underset{m1}{t} \tag{47}$$

the solution is given by

$$\begin{pmatrix} \underset{n1}{a} \\ \cdots \\ \underset{m1}{o} \end{pmatrix} = \begin{pmatrix} \underset{nm}{\tilde{F}} \\ \cdots \\ \mu \underset{mm}{I} \end{pmatrix} \cdot \left[\left(\underset{mn}{F} \,\vdots\, \mu \underset{mm}{I}\right) \cdot \begin{pmatrix} \underset{nm}{\tilde{F}} \\ \cdots \\ \mu \underset{mm}{I} \end{pmatrix} \right]^{-1} \cdot \underset{m1}{h} \tag{48}$$

which is the same as

$$\begin{pmatrix} \underset{n1}{a} \\ \cdots \\ \underset{m1}{o} \end{pmatrix} = \begin{pmatrix} \underset{nm}{\tilde{F}} \\ \cdots \\ \mu \underset{mm}{I} \end{pmatrix} \cdot \left(\underset{mn}{F} \cdot \underset{nm}{\tilde{F}} + \mu^2 \underset{mm}{I} \right)^{-1} \cdot \underset{m1}{h} \tag{49}$$

and (49) splits up into

$$\underset{nl}{a} = \underset{nm}{\tilde{F}} \cdot \left(\underset{mn}{F} \cdot \underset{nm}{\tilde{F}} + \mu^2 \underset{mm}{I} \right)^{-1} \cdot \underset{ml}{b} \qquad (50)$$

and

$$\underset{ml}{\overset{\circ}{a}} = \mu \left(\underset{mn}{F} \cdot \underset{nm}{\tilde{F}} + \mu^2 \underset{mm}{I} \right)^{-1} \cdot \underset{ml}{b} \qquad (51)$$

$\underset{nl}{a}$ given by (50) is the Tychonov solution to the INVERSION problem, and $\underset{ml}{a}$ given by (51) gives the non-zero residual which has had to be accepted as trade-off against the nicer properties of $(\underset{mn}{F} \cdot \underset{nm}{\tilde{F}} + u^2 \underset{mm}{I})^{-1}$ as compared with $(\underset{mn}{F} \cdot \underset{nm}{\tilde{F}})^{-1}$.

It is also found, by putting the SVD factorization into (50) that we come to exactly the same conclusion as in the analysis case, namely that the Tychonov solution is an approximation to the SVD solution.

Besides these well-known Tychonov solutions to the analysis and inversion problems it is possible to derive an Extended Tychonov solution to both problems.

In the ANALYSIS problem ($m > n$) instead of solving (39) to get the simple Tychonov solution we first factorize the $\left(\begin{smallmatrix} F \\ \mu I \end{smallmatrix}\right)$ matrix, using the Gram-Schmidt decomposition to get

$$\begin{pmatrix} \underset{mn}{F} \\ \hline \underset{mn}{\mu I} \end{pmatrix} = \begin{pmatrix} \underset{mn}{N} \\ \hline \underset{nn}{\tilde{S}} \end{pmatrix} \cdot \underset{nn}{C} \qquad (52)$$

This partitioned equation (52) yields the two relationships

$$\underset{mn}{N} \cdot \underset{nn}{C} = \underset{mn}{F} \qquad (53)$$

$$\underset{nn}{\tilde{S}} \cdot \underset{nn}{C} = \mu \underset{nn}{I} \qquad (54)$$

and from (54) we note the important fact that

$$\underset{nn}{\tilde{S}} = \mu \underset{nn}{C}^{-1} \qquad (55)$$

and now in place of (39) we solve the system

$$\begin{pmatrix} \underset{nn}{C} \\ \hline \underset{nn}{S} \end{pmatrix} \cdot \underset{nl}{a} = \begin{pmatrix} \underset{nm}{\tilde{N}} & ! & \underset{nn}{O} \\ \hline \underset{mn}{O} & ! & \underset{nn}{S} \end{pmatrix} \cdot \begin{pmatrix} \underset{ml}{h} \\ \hline \underset{nl}{o} \end{pmatrix} + \underset{nl}{t} \qquad (56)$$

The Normal Equations for (56) are

$$\left(\underset{nn}{\tilde{C}} \; ! \; \underset{nn}{\tilde{S}} \right) \cdot \begin{pmatrix} \underset{nn}{C} \\ \hline \underset{nn}{S} \end{pmatrix} \cdot \underset{nl}{a} = \left(\underset{nn}{\tilde{C}} \; ! \; \underset{nn}{\tilde{S}} \right) \cdot \begin{pmatrix} \underset{nm}{\tilde{N}} \cdot \underset{ml}{h} \\ \hline \underset{nl}{o} \end{pmatrix} \qquad (57)$$

i.e.

$$\left(\underset{nn}{\tilde{C}} \cdot \underset{nn}{C} + \underset{nn}{\tilde{S}} \cdot \underset{nn}{S} \right) \cdot \underset{nl}{a} = \underset{nn}{\tilde{C}} \cdot \underset{nm}{\tilde{N}} \cdot \underset{ml}{h} \qquad (58)$$

and, using the relationships above, this can be transformed back into

$$\left[\underset{nm}{\tilde{F}}\cdot\underset{mn}{F}+\mu^2\underset{nn}{I}+\mu^2\left(\underset{nm}{\tilde{F}}\cdot\underset{mn}{F}+\mu^2\underset{nn}{I}\right)^{-1}\right]\cdot\underset{n1}{a}=\underset{nm}{\tilde{F}}\cdot\underset{m1}{h} \tag{59}$$

which yields the Extended Tychonov solution

$$\underset{n1}{a}=\left[\underset{nm}{\tilde{F}}\cdot\underset{mn}{F}+\mu^2\underset{nn}{I}+\mu^2\left(\underset{nm}{\tilde{F}}\cdot\underset{mn}{F}+\mu^2\underset{nn}{I}\right)^{-1}\right]^{-1}\cdot\underset{nm}{\tilde{F}}\cdot\underset{m1}{h} \tag{60}$$

Now if we put the SVD factorization of F into (60) we get

$$\underset{n1}{a}=\left[\underset{nn}{V}\cdot\underset{nn}{\Lambda^2}\cdot\underset{nn}{\tilde{V}}+\mu^2\underset{nn}{V}\cdot\underset{nn}{\tilde{V}}+\mu^2\left(\underset{nn}{V}\cdot\underset{nn}{\Lambda}\cdot\underset{nn}{\tilde{V}}+\mu^2\underset{nn}{V}\cdot\underset{nn}{\tilde{V}}\right)^{-1}\right]^{-1}\cdot\underset{nn}{V}\cdot\underset{nn}{\Lambda}\cdot\underset{nm}{\tilde{U}}\cdot\underset{m1}{h}$$

which, with $V\cdot\underline{a}=\underline{b}$, reduces to

$$\underset{n1}{b}=\left[\underset{nn}{\Lambda^2}+\mu^2\underset{nn}{I}+\mu^2\left(\underset{nn}{\Lambda^2}+\mu^2 I\right)^{-1}\right]^{-1}\cdot\underset{nn}{\Lambda}\cdot\underset{nm}{\tilde{U}}\cdot\underset{m1}{h} \tag{61}$$

and, componentwise, this can be expressed as

$$b_j=\frac{\lambda_j}{\lambda_j^2+\mu^2+\dfrac{\mu^2}{\lambda_j^2+\mu^2}}\left(\underline{\tilde{u}}_j\cdot\underline{h}\right) \tag{62}$$

Comparing (62) with (45) we see that if μ is chosen so that the simple Tychonov regularization gives a good approximation to the SVD solution then the Extended Tychonov regularization (60) will be a closer approximation.

In the INVERSION problem ($m<n$) we can also derive an Extended Tychonov Regularization. Instead of solving (47) as it stands we first factorize using Gram-Schmidt to get

$$\left(\underset{mn}{F}\,\vdots\,\mu\underset{mm}{I}\right)=\underset{mm}{C}\cdot\left(\underset{mn}{N}\,\vdots\,\underset{mm}{\tilde{S}}\right) \tag{63}$$

from which we have

$$\underset{mm}{C}\cdot\underset{mn}{N}=\underset{mn}{F} \tag{64}$$

$$\underset{mm}{C}\cdot\underset{mm}{\tilde{S}}=\mu\underset{mm}{I} \tag{65}$$

and

$$\underset{mm}{\hat{S}}=\mu\underset{mm}{C^{-1}} \tag{66}$$

Then in place of (47) we solve

$$\left(\underset{mm}{C}\,\vdots\,\underset{mm}{S}\right)\cdot\begin{pmatrix}\underset{mn}{N} & \vdots & \underset{mm}{O}\\ \cdots & \cdots & \cdots\\ \underset{mm}{O} & \vdots & \underset{mm}{\tilde{S}}\end{pmatrix}\cdot\begin{pmatrix}\underline{a}\\ \cdots\\ \underline{a}\end{pmatrix}_{n1}=\underset{m1}{h} \tag{67}$$

the solution being (compare with (10) and (16))

$$\left(\begin{array}{c|c} \underset{mm}{N} & \underset{mm}{O} \\ \hline \underset{mm}{O} & \underset{mm}{\tilde{S}} \end{array}\right) \cdot \left(\begin{array}{c} \underset{nl}{a} \\ \hline \underset{ml}{\mathring{a}} \end{array}\right) = \left(\begin{array}{c} \underset{mm}{\tilde{C}} \\ \hline \underset{mm}{\tilde{S}} \end{array}\right) \cdot \left[\left(\underset{mm}{C} \,|\, \underset{mm}{S}\right) \cdot \left(\begin{array}{c} \underset{mm}{\tilde{C}} \\ \hline \underset{mm}{\tilde{S}} \end{array}\right)\right]^{-1} \cdot \underset{ml}{h} \tag{68}$$

which is

$$\left(\begin{array}{c|c} \underset{mm}{N} & \underset{mm}{O} \\ \hline \underset{mm}{O} & \underset{mm}{\tilde{S}} \end{array}\right) \cdot \left(\begin{array}{c} \underset{nl}{a} \\ \hline \underset{ml}{\mathring{a}} \end{array}\right) = \left(\begin{array}{c} \underset{mm}{\tilde{C}} \\ \hline \underset{mm}{\tilde{S}} \end{array}\right) \cdot \left(\underset{mm}{C} \cdot \underset{mm}{\tilde{C}} + \underset{mm}{S} \cdot \underset{mm}{\tilde{S}}\right)^{-1} \cdot \underset{ml}{h} \tag{69}$$

As stated in (ii), following (16), the algebra of the INVERSION case is trickier than that of the ANALYSIS case, but (69) can be solved explicitly for $\underset{nl}{a}$. By multiplying through by $\left(\begin{array}{c|c} \hat{N} & O \\ \hline O & S \end{array}\right)$ we arrive, after some reduction, at

$$\left(\begin{array}{c} \underset{nl}{a} \\ \hline \underset{ml}{\mathring{a}} \end{array}\right) = \left(\begin{array}{c|c} \underset{nm}{\tilde{N}} \cdot \underset{mm}{\tilde{C}} & \\ \hline \underset{mm}{S} \cdot \underset{mm}{\tilde{S}} & \end{array}\right) \cdot \left(\underset{mm}{C} \cdot \underset{mm}{\tilde{C}} + \underset{mm}{S} \cdot \underset{mm}{\tilde{S}}\right)^{-1} \cdot \underset{ml}{h} \tag{70}$$

which splits up into

$$\underset{nl}{a} = \left(\underset{nm}{\tilde{N}} \cdot \underset{mm}{\tilde{C}}\right) \cdot \left(\underset{mm}{C} \cdot \underset{mm}{\tilde{C}} + \underset{mm}{S} \cdot \underset{mm}{\tilde{S}}\right)^{-1} \cdot \underset{ml}{h} \tag{71}$$

$$\underset{ml}{\mathring{a}} = \left(\underset{mm}{S} \cdot \underset{mm}{\tilde{S}}\right) \cdot \left(\underset{mm}{C} \cdot \underset{mm}{\tilde{C}} + \underset{mm}{S} \cdot \underset{mm}{\tilde{S}}\right)^{-1} \cdot \underset{ml}{h} \tag{72}$$

and by using (64), (65), and (66) these are transformed back to

$$\underset{nl}{a} = \underset{nm}{\tilde{F}} \cdot \left[\underset{mm}{F} \cdot \underset{mm}{\tilde{F}} + \mu^2 \underset{mm}{I} + \mu^2 \left(\underset{mm}{F} \cdot \underset{mm}{\tilde{F}} + \mu^2 \underset{mm}{I}\right)^{-1}\right]^{-1} \cdot \underset{ml}{h} \tag{73}$$

$$\underset{ml}{\mathring{a}} = \mu^2 \left[\underset{mm}{F} \cdot \underset{mm}{\tilde{F}} + \mu^2 \underset{mm}{I} + \mu^2 \left(\underset{mm}{F} \cdot \underset{mm}{\tilde{F}} + \mu^2 \underset{mm}{I}\right)^{-1}\right]^{-1} \cdot \underset{ml}{h} \tag{74}$$

(73) gives $\underset{nl}{a}$ the sought for Extended Tychonov solution and (74) gives $\underset{ml}{a}$, the non-zero residual which has had to be accepted as a trade-off in return for the better behaved Extended Tychonov solution. Again, we can put the SVD decomposition into (73) and arrive after some algebra at exactly the same formula (62) for the b_j as given by the analysis case. And, of course the same conclusion can be drawn - if μ is chosen so that the simple Tychonov is a good approximation to the SVD solution then the Extended Tychonov will be a closer approximation.

3. The Assimilation Problem

It is probably true to say that but for the advent of SIRS data, with the promise of more and better HIRS to come, there would be no great pressure to tackle the difficult 4-d data analysis problem, because the amount of off-time data to

be available in the foreseeable future would scarcely justify the effort. In the absence of satellites a properly 4-d data problem would arise only if the world's governments could be persuaded to stagger their sondes in time and to increase the number of them to compensate for the consequent spatial thinning. If this were the position then we would have only one kind of problem. As it is, with SIRS and HIRS and sondes we have both kinds of problem in relation to assimilation. The point of Section 2 is that by clearly demonstrating the existence of a unified mathematical approach it brings to mind the possibility of organizing the assimilation problem in such a way that satellite and sonde information is dealt with in a unified way. At the moment the inversion, analysis, and assimilation procedures being developed are somewhat separate and this may be detrimental to their combination as a whole.

Thus the proposal is that a 4-d assimilation method should be sought in which the satellite radiances, the sonde heights and the model forecast fields are processed by a uniform technique which does not involve disparate sections.